

Analytic solution for heat flow through a general harmonic network

Nahuel Freitas^{1,2} and Juan Pablo Paz^{1,2}

¹*Departamento de Física, FCEyN, UBA, Pabellón 1,
Ciudad Universitaria, 1428 Buenos Aires, Argentina*

²*Instituto de Física de Buenos Aires, UBA CONICET,
Pabellón 1, Ciudad Universitaria, 1428 Buenos Aires, Argentina*

(Dated: June 9, 2015)

We present an analytic expression for the heat current through a general harmonic network coupled with Ohmic reservoirs. We use a method that enables us to express the stationary state of the network in terms of the eigenvectors and eigenvalues of a generalized cubic eigenvalue problem. In this way, we obtain exact formulas for the heat current and the local temperature inside the network. Our method does not rely on the usual assumptions of weak coupling to the environments or on the existence of an infinite cutoff in the environmental spectral densities. We use this method to study nonequilibrium processes without the weak coupling and Markovian approximations. As a first application, we revisit the problem of heat conduction in two- and three-dimensional crystals with binary mass disorder. We complement previous results showing that for small systems the scaling of the heat current with the system size greatly depends on the strength of the interaction between system and reservoirs. This somewhat counterintuitive result seems not to have been noticed before.

PACS numbers:

I. INTRODUCTION

The study of open quantum systems is important in many areas of current research. From a fundamental point of view, microscopic models of quantum open systems have been used to explore the quantum to classical transition and the emergence of thermodynamical laws [1–4]. These models are also of practical relevance for the study of the impact of decoherence on quantum devices, the quantum computer being the one that received the most attention recently [5–9]. Another area of fundamental and practical relevance related to open quantum systems is the study of energy transport, which is the main focus of this article.

The Caldeira-Leggett model for quantum Brownian motion (QBM) is the paradigmatic model of a quantum open system [3]. In this model the system consists of a single harmonic oscillator, which bilinearly interacts with a thermal reservoir formed by a set of uncoupled harmonic oscillators. The simplicity of the model allows for an analytical treatment, which has been used to obtain an exact master equation describing the evolution of the state of the system [10]. A similar analysis of the QBM model was recently generalized to the case where the system consists of an arbitrary network of harmonic oscillators which is connected with an arbitrary number of independent reservoirs [1]. This generalized QBM model can therefore be employed to study nonequilibrium phenomena and energy transport in complex quantum networks.

In this paper we build on the previous work [1] to obtain a simple analytic expression for the asymptotic stationary state of an arbitrary harmonic network coupled with Ohmic reservoirs. The stationary state is fully characterized by its covariance matrix containing all two-

point correlations of the network. Thus, we show that when all the reservoirs connected with the system are Ohmic, such covariance matrix can be simply expressed in terms of the eigenvalues and eigenvectors of a cubic eigenvalue problem. We show how to solve such generalized eigenvalue problem by transforming it into an ordinary linear one, which can be solved using rather standard techniques. It is important to stress that our solution is valid for arbitrary values of the system-reservoir coupling and for arbitrary cutoffs in the environmental spectral densities. Therefore, the method can be applied beyond the weak coupling and Markovian approximations.

Using our new method, we find a closed-form expression for the heat current through the system. This formula is a relevant result on its own. In fact, it enables us to study the energy transport through the network without appealing to methods based on Langevin dynamics which typically employ the Markovian approximation (assuming reservoirs with infinite high frequency cutoff) [11–17]. The complexity of the method is simply the one corresponding to finding eigenvalues and eigenvectors of a $3K \times 3K$ matrix (where K is the number of degrees of freedom of the network).

As a first application of our results, we revisit the problem of heat conduction and emergence of Fourier's Law in mass-disordered harmonic crystals. This problem has a long history, starting with the seminal work of Rieder, Lebowitz, and Lieb [11] and their observation of anomalous heat conduction. We show that the scaling of the heat current with system size is modified by the strength of the interaction between system and reservoirs. This is not expected if it is assumed, as in [12], that the localization of the normal modes of the closed system is enough to explain the effects of disorder on the transport properties of harmonic crystals. As we show here, that is not

the case. The scaling of the heat current with system size is completely different in the weak and strong coupling regimes.

The paper is organized as follows. In Sec. II we describe the model and the main results obtained in [1]. In Sec. III we show that when the network is coupled with Ohmic environments, its Green's function can be expressed in terms of the eigenvalues and eigenvectors of a cubic eigenvalue problem. We also use that result to obtain analytical formulas for the asymptotic state of the network and for heat currents. In Sec. IV A we show how the same techniques can be used in the limit of infinite cutoff. In this simpler case, all relevant quantities are expressed in terms of the solution of a quadratic eigenvalue problem. In Sec. IV B we analyze an even simpler regime showing that in the weak coupling limit both the state and the heat current can be obtained from the regular normal modes and frequencies of the closed system. We also give a general proof of the anomalous scaling of the heat flow in harmonic systems. Finally, in Sec. V the previous results are applied to the study of the scaling of the heat current in two-dimensional (2D) 3D crystals with binary mass disorder.

II. DESCRIPTION OF THE MODEL

We consider a system of K harmonic oscillators with arbitrary bilinear interactions, whose dynamics is described by the Hamiltonian

$$H_S = \frac{1}{2} (P^T M^{-1} P + X^T V X), \quad (1)$$

where $P = (p_1, \dots, p_K)^T$ and $X = (x_1, \dots, x_K)^T$ are vectors formed with the momentum and position operators of each oscillator, while M and V are the mass and interaction matrices describing the harmonic network. We consider $\hbar = 1$, so $[x_k, p_{k'}] = i\delta_{k,k'}$. The system is coupled in a linear way to several bosonic reservoirs which are initially in a thermal state. The total Hamiltonian is then $H_T = H_S + H_E + H_{int}$. The environmental Hamiltonian is $H_E = \sum_l H_l$, where H_l is the Hamiltonian of the l -th reservoir:

$$H_l = \frac{1}{2} \sum_j \frac{(\pi_j^l)^2}{m_j^l} + m_j^l (\omega_j^l)^2 (q_j^l)^2. \quad (2)$$

The operators π_j^l and q_j^l are such that $[q_j^l, \pi_{j'}^{l'}] = i\delta_{j,j'}\delta_{l,l'}$. The interaction between the system and the reservoirs is described by

$$H_{int} = \sum_{l,j,k} C_{k,j}^l x_k q_j^l, \quad (3)$$

where $C_{k,j}^l$ are arbitrary real interaction constants.

Initially, the reservoirs are in thermal states ρ_{th}^l (with arbitrary temperatures) and are uncorrelated with the

system; i.e., the total density matrix is $\rho_T|_{t=0} = \rho_S \otimes \rho_E$, with $\rho_E = \otimes_l \rho_{th}^l$. We are interested in the subsequent evolution of the reduced state of the system $\rho_S = Tr_E(\rho_{SE})$ which, as explained in [1], obeys a linear and time-local master equation with time-dependent coefficients. The interaction with the reservoirs induce non unitary effects over the system such as diffusion and dissipation, as well as a unitary renormalization of the system's Hamiltonian. The only relevant properties of each reservoir are the temperature and the spectral density, defined as $I_{k,k'}^l = \sum_j C_{k,j}^l C_{k',j}^l \delta(\omega - \omega_j^l) / (2m_j^l \omega_j^l)$. Thus, $I^l(\omega)$ are $K \times K$ real and symmetric matrices. The total spectral density is $I(\omega) = \sum_l I^l(\omega)$. Two relevant functions are defined in terms of the spectral densities: the dissipation kernel $\gamma(t) = \int_0^\infty I(\omega) \cos(\omega t) d\omega$ and the noise kernel $\nu(t) = \int_0^\infty \sum_l I^l(\omega) \coth(\omega/2T_l) \cos(\omega t) d\omega$, where T_l is the temperature of the l -th reservoir (the Boltzmann constant is set to 1).

A complete description of the instantaneous state of the system is given by the characteristic function $\chi(\alpha, t) = Tr(\rho(t) e^{-i(Py - Xk)})$, where $\alpha = (k, y)^T$ is a $2K$ -component vector containing the displacement in phase space. It can be shown that the evolution of χ satisfies[1]

$$\chi(\alpha, t) = \chi(\Phi(t)^T \alpha, 0) e^{-\frac{1}{2} \alpha^T \Sigma(t) \alpha}. \quad (4)$$

The time dependence is contained in the $2K \times 2K$ matrices $\Phi(t)$ and $\Sigma(t)$. Therefore, the evolution of the system consists of a phase space flow (given by $\Phi(t)$) combined with a Gaussian modulation [given by $\Sigma(t)$]. $\Phi(t)$ and $\Sigma(t)$ can be obtained from the Green's function of the system, $G(t)$, which in turn satisfies an integro-differential equation,

$$M\ddot{G}(t) + V_R G(t) + 2 \int_0^t \gamma(t-\tau) \dot{G}(\tau) d\tau = 0, \quad (5)$$

with initial conditions $G(0) = 0$ and $\dot{G}(0) = M^{-1}$. $V_R = V - 2\gamma(0)$ is the renormalized potential. In terms of $G(t)$, we have

$$\Phi(t) = \begin{bmatrix} \dot{G}(t) & G(t) \\ \ddot{G}(t) & \dot{G}(t) \end{bmatrix}, \quad \Sigma(t) = \begin{bmatrix} \sigma^{xx}(t) & \sigma^{xp}(t) \\ \sigma^{px}(t) & \sigma^{pp}(t) \end{bmatrix}, \quad (6)$$

where $\sigma^{xx} = \sigma^{(0,0)}$, $\sigma^{pp} = \sigma^{(1,1)}$, and $\sigma^{xp} = \sigma^{(0,1)}$, with

$$\sigma^{(n,m)}(t) = \int_0^t \int_0^t G^{(n)}(t_1) \nu(t_1 - t_2) G^{(m)}(t_2) dt_1 dt_2, \quad (7)$$

where $G^{(n)}$ is the n -th derivative of G . We consider the case in which the reservoirs consist of a dense distribution of harmonic oscillators and the spectral density can be modeled as a continuous function of ω . In that case the induced diffusion and dissipation will drive the system to a Gaussian stationary state. The covariance matrix of that stationary state is just $\Sigma = \lim_{t \rightarrow \infty} \Sigma(t)$, as can be seen from Eq. (4). The blocks of Σ can be expressed as the following integral in the frequency domain:

$$\sigma^{(n,m)} = Re \int_0^\infty \omega^{n+m} i^{n-m} \hat{G}(i\omega) \hat{\nu}(w) \hat{G}(-i\omega) d\omega. \quad (8)$$

In the previous expression, $\sigma_{i,j}^{(0,0)} = \langle x_i x_j \rangle$, $\sigma_{i,j}^{(0,1)} = \langle x_i p_j \rangle$, $\sigma_{i,j}^{(1,1)} = \langle p_i x_j \rangle$, and $\sigma_{i,j}^{(1,1)} = \langle p_i p_j \rangle$ are the two-point correlations functions in the asymptotic state. Also, $\hat{\nu}(\omega)$ is the Fourier transform of the noise kernel. The main ingredient that enters into the above expression is $\hat{G}(s)$, the Laplace transform of the Green's function, which satisfies

$$\hat{G}(s) = (s^2 M + V_R + 2s\hat{\gamma}(s))^{-1}, \quad (9)$$

where $\hat{\gamma}(s)$ is the Laplace transform of the dissipation kernel.

Now we turn to the analysis of the heat flow through the system. The mean value of the power injected by the l -th reservoir into the system is $\dot{Q}_l = \text{Tr}(P_l V_R \sigma^{(0,1)})$ [1], where P_l is a projector over the sites of the network in contact with the corresponding reservoir. In the stationary limit the conservation law $\sum_l \dot{Q}_l = 0$ is satisfied, while, in general $\sum_l \dot{Q}_l = \frac{d}{dt} \langle H_R \rangle$, where H_R is the renormalized Hamiltonian (see [1] for details). Using Eq. (8) to express $\sigma^{(0,1)}$, the following expression is obtained:

$$\begin{aligned} \dot{Q}_l = \sum_{l'} \text{Im} \int_0^\infty \omega d\omega \coth(\omega/2T_{l'}) \\ \times \text{Tr}(P_l V_R \hat{G}(i\omega) I_{l'}(\omega) \hat{G}^\dagger(i\omega)). \end{aligned} \quad (10)$$

From this equation we can see that \dot{Q}_l is a sum over all the environments,

$$\dot{Q}_l = \sum_{l'} \int_0^\infty \omega d\omega \dot{Q}_{ll'}(\omega) \coth(\omega/2T_{l'}), \quad (11)$$

where the heat transfer matrix \dot{Q} is defined as

$$\dot{Q}_{ll'}(\omega) = \text{Im} \text{Tr}(P_l V_R \hat{G}(i\omega) I_{l'}(\omega) \hat{G}^\dagger(i\omega)). \quad (12)$$

Using the equation for $\hat{G}(s)$ it is possible to show that the heat transfer matrix is such that $\sum_l \dot{Q}_{ll'} = 0$ and that, for $l \neq l'$,

$$\dot{Q}_{ll'}(\omega) = -\pi \text{Tr}(I_l(\omega) \hat{G}(i\omega) I_{l'}(\omega) \hat{G}^\dagger(i\omega)). \quad (13)$$

Using now this equation we can rewrite the heat flow from the l -th reservoir as follows:

$$\dot{Q}_l = - \sum_{l' \neq l} \int_0^\infty \omega d\omega \dot{Q}_{ll'}(\omega) (\coth(\omega/2T_l) - \coth(\omega/2T_{l'})) \quad (14)$$

This is the expression we use to compute the heat flow. From it, we can see that the heat flow is a bilinear functional of $\hat{G}(s)$.

All the previous results are valid for reservoirs with arbitrary spectral densities. However, in the rest of this article we consider the particular case in which all the reservoirs are Ohmic and their spectral densities have the same Lorentz-Drude cutoff, i.e., $I^l(\omega) = \frac{2}{\pi} \gamma_0 P_l \frac{\omega \Lambda^2}{\omega^2 + \Lambda^2}$, where P_l is a projector over the sites of the network

which are in contact with the l -th reservoir. Moreover, γ_0 controls the strength of the coupling, and Λ is a high frequency cutoff. In this case, the Laplace transform of the dissipation kernel is $\hat{\gamma}(s) = \gamma_0 \frac{\Lambda}{s + \Lambda} \sum_l P_l$ and the Fourier transform of the noise kernel is $\hat{\nu}(\omega) = \sum_l I^l(\omega) \coth(\frac{\omega}{2T_l})$. Finally, the renormalized potential is $V_R = V - \Delta V$ with $\Delta V = \gamma_0 \Lambda \sum_l P_l$.

In the following sections we show how to perform the frequency integrals Eqs. (8) and (14) analytically. We obtain closed-form expressions in terms of the eigenvalues and eigenvectors of a cubic eigenvalue problem related to the inversion of $\hat{G}^{-1}(s)$.

III. RELATION TO THE CUBIC EIGENVALUE PROBLEM

It is straightforward to see that when all the environments are Ohmic and have the same cutoff, the Laplace transform of the Green's function can be expressed as

$$\hat{G}(s) = (s + \Lambda) g(s)^{-1}, \quad (15)$$

where $g(s)$ is a $K \times K$ matrix which depends polynomially on s and satisfies

$$g(s) = s^3 M + s^2 \Lambda M + s(V + \Delta V) + \Lambda(V - \Delta V). \quad (16)$$

Therefore, to compute $\hat{G}(s)$ one needs to obtain $g(s)^{-1}$ and for this purpose we need to invert the cubic matrix polynomial that defines $g(s)$. The inversion of such matrix is related to the solution of the cubic eigenvalue problem defined by $g(s)$. The cubic eigenvalue problem consists of finding the generalized eigenvalues $\{s_\alpha\}$ and eigenvectors $\{r_\alpha\}$ that satisfy the equations:

$$\det(g(s_\alpha)) = 0 \quad \text{and} \quad g(s_\alpha) r_\alpha = 0. \quad (17)$$

As $\det(g(s))$ is a $3K$ degree polynomial in s then it has $3K$ complex roots $\{s_\alpha\}$. Moreover, as the matrix coefficients appearing in $g(s)$ are real, the eigenvalues $\{s_\alpha\}$ come in complex conjugate pairs. In Appendix A we show that the inverse of $g(s)$ can be written as

$$g(s)^{-1} = \sum_{\alpha=1}^{3K} \frac{r_\alpha l_\alpha^\dagger}{s - s_\alpha}, \quad (18)$$

where $\{r_\alpha\}_{\alpha=1 \dots 3K}$ and $\{l_\alpha\}_{\alpha=1 \dots 3K}$ are K component column vectors that are obtained from the eigenvectors of a $3K \times 3K$ linear system. Equation (18) is crucial for the method we present in this paper. In fact, in Eq. (18), the inverse of $g(s)$ is expressed in terms of its poles, which are the eigenvalues $\{s_\alpha\}$. Thus, this expression can be used in the integrals which appear in Eqs. (8) and (14), which are central in computing the covariance matrix and heat currents of the asymptotic state. By doing this, all integrals can be analytically solved by appropriately choosing complex contours and using the residue theorem. In this way a final analytical result for the covariance matrix can

be obtained (and the final result does not involve any integral to be numerically evaluated, which is one of the typical major problems of other existing methods [16]).

As we show in Appendix B, it is possible to solve Eq. (8) by extending it to the complex plane and using the residue theorem. The result we obtain is:

$$\sigma^{(n,m)} = \sigma_H^{(n,m)} - \left(\sigma_L^{(n,m)} + (-1)^{n+m} [\sigma_L^{(n,m)}]^T \right), \quad (19)$$

where the matrices $\sigma_H^{(n,m)}$ and $\sigma_L^{(n,m)}$ are:

$$\sigma_{H,L}^{(n,m)} = 2\gamma_0 \Lambda^2 Re \left[i^{n-m+1} \sum_{\alpha,\beta=1}^{3K} \omega_\alpha^{n+m} \frac{l_\alpha^\dagger A_{H,L}(\omega_\alpha) r_\beta}{\omega_\alpha + \omega_\beta} r_\alpha l_\beta^\dagger \right]. \quad (20)$$

The eigenfrequencies ω_α are related to the poles of $g(s)^{-1}$: $\omega_\alpha = -is_\alpha$. The matrices A_H and A_L appearing in the previous expression are defined as:

$$\begin{aligned} A_H(\omega) &= \sum_l 2T_l P_l \\ A_L(\omega) &= \frac{\omega}{i\pi} \sum_l P_l \psi \left(1 - \frac{i\omega}{2\pi T_l} \right), \end{aligned} \quad (21)$$

where ψ is the digamma function. Equation (19) is a decomposition of the asymptotic covariance matrix in a term corresponding to the high temperature regime, $\sigma_H^{(n,m)}$, and a correction for low temperatures, given by $\sigma_L^{(n,m)}$. Equations (19) and (20) are the main results for this paper. In fact, by using these formulas one can fully determine the asymptotic state of an arbitrary network of harmonic oscillators coupled to several thermal environments by simply solving a linear eigenvalue problem. This solution is valid for arbitrary temperatures, coupling strength, and frequency cutoff.

The same integration technique can be applied to the integral of Eq. (14). The result is $\dot{Q}_l = \sum_{l' \neq l} \dot{q}_{l,l'}$, with

$$\dot{q}_{l,l'} = [2\gamma_0 \Lambda^2]^2 \sum_{\substack{\alpha,\beta=1 \\ \omega_\alpha \neq i\Lambda}}^{3K} \frac{\omega_\alpha^3 \Delta_{l,l'}(\omega_\alpha)}{\omega_\alpha^2 + \Lambda^2} \frac{(l_\beta^\dagger P_l r_\alpha)(l_\alpha^\dagger P_{l'} r_\beta)}{\omega_\alpha + \omega_\beta}, \quad (22)$$

where:

$$\begin{aligned} \Delta_{l,l'}(\omega) &= i \frac{2(T_l - T_{l'})}{\omega} - \\ &\quad - \frac{2}{\pi} \left[\psi \left(1 - \frac{i\omega}{2\pi T_l} \right) - \psi \left(1 - \frac{i\omega}{2\pi T_{l'}} \right) \right] \end{aligned} \quad (23)$$

As is evident from Eq. (22), it is not possible to express the heat current as a sum of independent contributions for each normal mode. This reflects in the fact that in the above expressions a double sum over modes appears instead of a single one. The terms with $\omega_\alpha \neq \omega_\beta^*$ correspond to interactions between different normal modes mediated by the common reservoirs. As a consequence, it

is not possible to classify the normal modes into ballistic or diffusive ones by analyzing their structure or scaling properties only. In other words, for any given value of the eigenfrequency, the energy transmission of the system does not depend only on the structure of the normal mode corresponding to that frequency, but also on the structure of all the other normal modes. However, as we show in the following section, in the weak coupling limit this situation changes. In that case it is indeed possible to write the heat current as a single sum of independent contributions that can be associated with individual normal modes.

IV. THREE SIMPLE APPLICATIONS: RECOVERING KNOWN RESULTS

In this Section we apply the method developed above to analyze some simple, well studied, limiting cases. Here we first discuss the case where all the environments have an infinitely large cutoff. Then we revisit the weak coupling limit recovering simple analytic expressions for the heat flow. Finally, we use the weak coupling results to prove that the heat transport is always anomalous for symmetric harmonic networks.

A. Environments with infinite cutoff frequency

Let us show how the technique presented above simplifies when the environments have an infinite high frequency cutoff (i.e., $\Lambda \rightarrow \infty$). This limit has to be taken with some care. On the one hand, it is known that the effect of a finite cutoff always shows up at short times after the preparation of a non-equilibrium initial state. Thus, our results could not be used to study such regime. Of course this is not a problem if we are interested in the study of the stationary behavior achieved for long times. On the other hand, when $\Lambda \rightarrow \infty$ the shift in the potential, ΔV , diverges. To deal with this, we must absorb the shift into a renormalization of the coupling matrix. Thus, we consider that the renormalized coupling matrix defined as $V_R = V - \Delta V$ is finite and carries all the information about the renormalized dynamics of the system.

In the limit of infinite cutoff, the spectral density is $I^l(\omega) \rightarrow \frac{2}{\pi} \gamma_0 P_l \omega$. Thus, in this limit the dissipation kernel becomes local, i.e., $\hat{\gamma}(s) \rightarrow \gamma_0 P_T$, where $P_T = \sum_l P_l$ carries the information about the sites coupled with the environments. Consequently, the Laplace transform of the Green's function, $\hat{G}(s)$, satisfies

$$\hat{G}(s) = (s^2 M + V_R + 2s\gamma_0 P_T)^{-1}. \quad (24)$$

This equation, in fact, has been extensively studied in the literature in the context of the study of transport phenomena in harmonic systems [15–17]. Below we show that using the method described above we can find a simple analytic solution.

In fact, using the techniques explained in [18] it is possible to show that $\hat{G}(s)$ can be written as

$$\hat{G}(s) = \sum_{\alpha=1}^{2K} \frac{s_{\alpha}}{s - s_{\alpha}} r_{\alpha} r_{\alpha}^T, \quad (25)$$

where s_{α} and r_{α} are such that

$$\hat{G}^{-1}(s_{\alpha}) r_{\alpha} = 0. \quad (26)$$

It is worth noting that in this case the Green's function is obtained as a sum over a set of $2K$ generalized modes. This is in contrast to the case with a finite cutoff where the number of generalized modes was $3K$. The reason for this is simple: when the cutoff is infinite, $\hat{G}^{-1}(s)$ is a quadratic matrix polynomial in s . Then, there are $2K$ eigenvalues s_{α} and eigenvectors r_{α} . Thus, for any finite cutoff we find $3K$ modes. However, K of them are such that in the $\Lambda \rightarrow \infty$ limit they decay with a rate proportional to Λ and, therefore, are frozen. As before, generalized eigenfrequencies and eigenmodes come in complex conjugate pairs since the matrix coefficients of $\hat{G}^{-1}(s)$ are real.

To find $\hat{G}(s)$ we must solve the quadratic eigenvalue problem. As before, this can be reduced to a linear eigenvalue problem in a space of higher dimension. Thus, a pair (s_{α}, r_{α}) satisfying Eq. (26) will also satisfy the equation

$$(s_{\alpha}B - A) \begin{bmatrix} r_{\alpha} \\ s_{\alpha}r_{\alpha} \end{bmatrix} = 0, \quad (27)$$

with

$$A = \begin{bmatrix} 0 & C \\ -V_R & -2\gamma_0 P_T \end{bmatrix}, \quad B = \begin{bmatrix} C & 0 \\ 0 & M \end{bmatrix}. \quad (28)$$

Here, C can be chosen as any invertible $K \times K$ matrix. Without losing generality, we choose $C = -V_R$ so that both A and B are symmetric matrices. In this case, left and right eigenvectors of the linear system are the same [and only one of them appear in Eq. (25)]. The eigenvectors r_{α} are chosen so that the normalization condition $R^T B R = \mathbf{1}$ holds, where the columns of R are the vectors $\begin{bmatrix} r_{\alpha} \\ s_{\alpha}r_{\alpha} \end{bmatrix}$.

The frequency integrals involved in the calculation of the heat flow can be solved following the same procedure described in the Appendix B. Therefore, Eq. 19 also applies for this case and the matrices $\sigma_H^{(n,m)}$ and $\sigma_L^{(n,m)}$ can be calculated as:

$$\sigma_{H/L}^{(n,m)} = 2\gamma_0 \text{Re} \left[i^{n-m-1} \sum_{\alpha,\beta=1}^{2K} \omega_{\alpha}^{n+m+1} \omega_{\beta} \frac{r_{\alpha}^T A_{H/L}(\omega_{\alpha}) r_{\beta}}{\omega_{\alpha} + \omega_{\beta}} r_{\alpha} r_{\beta}^T \right], \quad (29)$$

where, as before, $\omega_{\alpha} = -is_{\alpha}$ and $A_{H/L}(\omega)$ are defined by Eq. (21). It is important to note that Eq. 29 is not valid

to calculate $\sigma_L^{(1,1)}$. The reason is that for the case of an infinite cutoff the integrand of Eq. 8 goes as $\log(\omega)/\omega$ for $n = m = 1$ and low temperatures. It is therefore not possible to choose an integration path with a vanishing contribution at infinity. As a consequence, in the high cutoff limit it is not possible to use the same integration technique to evaluate the low temperature corrections for the momentum-momentum correlations.

The following expression is obtained for the heat currents in the high cutoff limit:

$$\dot{q}_{l,l'} = -4\gamma_0^2 \sum_{\alpha,\beta=1}^{2K} \Delta_{l,l'}(\omega_{\alpha}) \frac{\omega_{\alpha}^4 \omega_{\beta}}{\omega_{\alpha} + \omega_{\beta}} (r_{\alpha}^T P_l r_{\beta}) (r_{\beta}^T P_{l'} r_{\alpha}). \quad (30)$$

This is a simplified version of Eq. (22).

B. The weak coupling limit

The above formulas can be further simplified in the weak coupling limit. For this we expand all the expressions up to second order in the system-environment coupling constant (i.e., first order in γ_0). It is simple to show that in this limit we can use the expressions obtained above for the infinite cutoff case. Thus, we need to expand the generalized eigenvectors and eigenvalues of the quadratic eigenvalue problem presented in the previous subsection. Doing this we find

$$s_{\alpha} = \pm i\Omega_{\alpha} - \gamma_0 \frac{q_{\alpha}^T P_T q_{\alpha}}{q_{\alpha}^T M q_{\alpha}} \quad (31a)$$

$$r_{\alpha} = q_{\alpha} \mp 2i\gamma_0 \sum_{\beta \neq \alpha} q_{\beta} \frac{\Omega_{\alpha}}{\Omega_{\beta}^2 - \Omega_{\alpha}^2} \frac{q_{\beta}^T P_T q_{\alpha}}{q_{\beta}^T M q_{\beta}} \quad (31b)$$

In the above expressions Ω_{α} and q_{α} are the (positive) normal frequencies and their corresponding eigenvectors of the closed network (which is described by the mass and the coupling matrices M and V_R). The only subtle detail of this calculation is taking care of the normalization condition for the vectors q_{α} . Such vectors satisfy the condition $R^T B R = I$. This reads as $q_{\alpha}^T M q_{\beta} = \frac{-1}{2\omega_{\alpha}^2} \delta_{\alpha\beta}$. Therefore one can write these vectors as:

$$q_{\alpha} = \frac{i}{\sqrt{2}(\pm\Omega_{\alpha})} q_{\alpha}^0 \quad (32)$$

where $\{q_{\alpha}^0\}$ are real vectors satisfying the normalization condition $q_{\alpha}^{0T} M q_{\beta}^0 = \delta_{\alpha\beta}$.

Using this we can find the weak coupling form of the covariance matrix and the heat current, which in the general case are given by equations (29) and (30). Before doing this it is convenient to rewrite the above expressions using the notation $\omega_{\alpha} = \pm\Omega_{\alpha} + i\Gamma_{\alpha}$, where Ω_{α} and Γ_{α} real and positive numbers. Also, Γ_{α} is proportional to the coupling constant γ_0 . Therefore, when $\Gamma_{\alpha} \ll \min_{\alpha \neq \beta} |\Omega_{\alpha} \pm \Omega_{\beta}|$, we have that $(\omega_{\alpha} + \omega_{\beta})^{-1}$ is vanishingly small except when $\omega_{\alpha} = -\omega_{\beta}^*$. This result

implies that all modes decouple and contribute independently to the covariance matrix and the heat current. Thus, the double summations appearing both in (29) and in (30) are clearly dominated by the diagonal terms (i.e., when $\omega_\alpha = -\omega_\beta^*$). More explicitly,

$$\frac{1}{\omega_\alpha + \omega_\beta} = \begin{cases} \frac{1}{2i\Gamma_\alpha} & \text{if } \omega_\alpha = -\omega_\beta^* \\ \frac{1}{(\Omega_\alpha \pm \Omega_\beta) + i(\Gamma_\alpha + \Gamma_\beta)} & \text{if } s_\alpha \neq s_\beta^* \end{cases} \quad (33)$$

In this way we find that the high temperature covariance matrix is:

$$\sigma_H^{n,m} = \frac{\delta_{n,m}}{2} \sum_{\alpha=1}^K \Omega_\alpha^{n+m-1} K_\alpha q_\alpha^0 q_\alpha^{0T} + \mathcal{O}(\gamma_0), \quad (34)$$

with $K_\alpha = \frac{1}{q_\alpha^T P_T q_\alpha} \sum_l q_\alpha^T P_l q_\alpha \left(\frac{2T_l}{\omega_\alpha} \right)$. To find this, we used Eq. (31) and also the normalization condition of Eq. (32). Note that in equation (34) only the K normal modes q_α^0 and eigenfrequencies Ω_α of the closed systems appear.

Using the same approximations the following expression is obtained for the heat current:

$$\dot{q}_{l,l'} = \gamma_0 \sum_{\alpha=1}^K I_\alpha (-i\Omega_\alpha \Delta_{l,l'}(\Omega_\alpha)) + \mathcal{O}(\gamma_0^2) \quad (35)$$

with:

$$I_\alpha = \frac{(q_\alpha^{0T} P_l q_\alpha^0)(q_\alpha^{0T} P_{l'} q_\alpha^0)}{q_\alpha^{0T} P_l q_\alpha^0 + q_\alpha^{0T} P_{l'} q_\alpha^0} \quad (36)$$

This last expression is a measure of the thermal conduction between reservoirs l and l' of the normal mode α . Now we see that in the weak coupling limit the thermal conduction of a single normal mode can be analyzed and classified in terms of its structure and scaling properties only, in contrast with the strong coupling regime. An expression similar to equation (35) was first derived by Matsuda and Ishii in [14] working directly in the weak coupling limit and for a one-dimensional system. Here we have rederived it from a more general formula valid for arbitrary coupling strengths and network topology.

C. Heat transport is anomalous

We can now use the above results to present a simple and general proof of the fact that the heat transport through symmetric harmonic networks is always anomalous (as defined below). For this we will consider that the network is coupled to only two reservoirs A and B .

The derivation is particularly simple under the reasonable assumption of a symmetric coupling between the network and its environments. Specifically, we will assume that there exist an orthogonal matrix S , representing the symmetry operation, which transforms the mass and coupling matrices as

1. $M = S^T M S$
2. $V_R = S^T V_R S$
3. $P_A = S^T P_B S$

In this case, the eigenvectors q_α^0 can always be chosen so that $q_\alpha^{0T} P_A q_\alpha^0 = q_\alpha^{0T} P_B q_\alpha^0$. This can be used in equation (36), which now reduces to $I_\alpha = \frac{1}{2} q_\alpha^{0T} P_A q_\alpha^0 = \frac{1}{2} q_\alpha^{0T} P_B q_\alpha^0$.

Assuming that both environments are at high temperatures, the heat flow is then $\dot{q} = \gamma_0(T_A - T_B) \sum_{\alpha=1}^K q_\alpha^{0T} P_A q_\alpha^0$. The last sum is equal to $\text{Tr}(M^{-1} P_A)$. Then, if P_A is a projector over c sites of the harmonic network and the mass matrix is diagonal, the heat current is simply:

$$\dot{q} = c\gamma_0 \langle m^{-1} \rangle (T_A - T_B). \quad (37)$$

In this equation the symbol $\langle m^{-1} \rangle$ denotes the mean value of the inverse of the mass of the elements of the network which are coupled to the reservoirs. Therefore, the heat flow per site in contact with the reservoirs, which is $J = \dot{q}/c$, does not scale with the system size and does not depend on any internal detail of the network, as long as the symmetry condition is fulfilled. Of course, this is valid in the weak coupling limit.

The heat transport in symmetric harmonic networks is therefore anomalous, in the sense that it is not possible to define a size-independent (i.e., intensive) thermal conductivity. For a system satisfying Fourier's Law the thermal conductivity is defined as $\kappa = JL/\Delta T$, where J is the heat flow per unit area and L is the length of the system in the direction of heat conduction. From our results it follows that for any symmetric network the heat conductivity is proportional to L , for sufficiently weak coupling.

As far as we known, this is the most general proof of the anomalous scaling of heat flow in harmonic networks. Previous results were limited to ordered d -dimensional lattices with first neighbor interactions. [15, 19, 20].

V. HEAT FLOW IN THE STRONG COUPLING LIMIT. EMERGENCE OF FOURIER'S LAW AND ANDERSON LOCALIZATION

Here we will present the first non trivial application of our method, to study the heat transport through a network strongly coupled with two reservoirs at different temperatures. We will study the dependence of the heat flow with the size of the system for 2D and 3D cases. As heat conduction is always anomalous for harmonic networks, we will analyze the effect of static disorder and discuss the emergence of Fourier law, which is valid in the macroscopic domain. The emergence of Fourier's law has been extensively discussed in the literature. One of the mechanisms that could explain the emergence of such law

is Anderson localization which occurs in disordered harmonic crystals. In fact, a recent study [12], which claims to present the “first microscopic verification of Fourier’s Law in a three-dimensional system”, points in that direction. Here, we will revisit the same model analyzed in [12] and present numerical evidence that questions the conclusions of that work. In that paper, the authors numerically studied the size dependence of the heat current in 2D and 3D crystals with binary mass disorder.

We will study the heat current J , which is defined as the heat flow per unit area, i.e., $J = \dot{Q}/N'$, where $N' = N^{d-1}$ is the number of sites in contact with each reservoir in a lattice of d dimensions and N^d sites. The heat current typically scales with the size of the system as a power law:

$$J \propto \frac{1}{N^\mu} \quad (38)$$

where N is the length of the system in the direction of heat conduction. For the Fourier Law to be valid we need $\mu = 1$. To the contrary, as we showed in section IV C, for symmetric networks in the weak coupling limit we always find that the heat transport is anomalous with $\mu = 0$.

In [12] a careful study of the dependence of μ with dimensionality of the system and on the boundary conditions was presented. Their conclusion is that for 3D systems with binary mass disorder one can expect that $\mu = 1$, a result that is consistent with Fourier’s law. However, as we will see below, this result is strongly dependent on the value of the coupling constant between the crystals and the reservoirs. In fact, in [12] the dependence of μ on γ_0 was not analyzed (thus, the authors explicitly mentioned that “the value of μ will not depend on γ_0 ”). As we show below, this is not the case. On the contrary, we find a strong dependence of μ on γ_0 . We show that disordered 3D crystals also display anomalous transport for weak coupling (i.e., $\mu = 0$). Instead, in the strong coupling regime such crystals have non vanishing values of μ , which strongly depend on γ_0 . Thus, our results indicate that the effect of disorder on the transport properties of harmonic crystals cannot be fully understood in terms of the localization of the normal modes of the isolated system. The strong interaction with the reservoirs seems to play a crucial role.

The model we will analyze is defined by the Hamiltonian considered in [12], which is:

$$H = \frac{1}{2} \sum_{\hat{n}} m_{\hat{n}} \dot{x}_{\hat{n}}^2 + k_0 x_{\hat{n}}^2 + \frac{1}{2} \sum_{\hat{n}, \hat{e}} (x_{\hat{n}} - x_{\hat{n}+\hat{e}})^2, \quad (39)$$

where \hat{n} labels the sites of a d -dimensional hypercubic lattice with N^d sites. In turn, \hat{e} labels the $2d$ nearest-neighbors which are coupled with any given site \hat{n} . This type of system can therefore be divided in N slabs, each one of which has $N' = N^{d-1}$ sites. We assume that the first and the last slab of the crystal are connected to two independent reservoirs at different temperatures T_A and T_B . The coupling constant appearing in the spectral

density of the reservoirs is γ_0 . In this model, disorder is introduced by setting the masses of half of the sites (randomly selected) to $\bar{m} + \Delta$ and the other half to $\bar{m} - \Delta$. In the following we set the values of the internal coupling constants and the masses to be $k = 1$ and $\bar{m} = 1$. Also, we will only consider pinned lattices, i.e., $k_0 \neq 0$. We will only present results corresponding to high temperatures. In such case, the heat current is proportional to the temperature difference $\Delta T = T_A - T_B$.

To obtain the heat current for a given configuration we solved numerically the eigenvalue problem given in Eq. (27):

$$\left(s_\alpha \begin{bmatrix} -V_R & 0 \\ 0 & M \end{bmatrix} + \begin{bmatrix} 0 & V_R \\ V_R & 2\gamma_0 P_T \end{bmatrix} \right) \begin{bmatrix} r_\alpha \\ s_\alpha r_\alpha \end{bmatrix} = 0 \quad (40)$$

Where $M = \text{diag}(m_1, m_2, \dots, m_{N^d})$ and the matrices V_R and P_T exhibit the following tridiagonal block structure:

$$V_R = \begin{bmatrix} v & -\mathbb{1} & & \\ -\mathbb{1} & v & -\mathbb{1} & \\ & & \ddots & \\ & & -\mathbb{1} & v & -\mathbb{1} \\ & & & -\mathbb{1} & v \end{bmatrix} \quad P_T = \begin{bmatrix} \mathbb{1} & & & \\ & 0 & & \\ & & \ddots & \\ & & & 0 \\ & & & & \mathbb{1} \end{bmatrix} \quad (41)$$

In the previous expression for V_R the $N^{d-1} \times N^{d-1}$ matrix v contains the couplings of an internal slab (note that all the slabs are equal, since the couplings are uniform and only the masses are disordered). In turn, the matrix v also has a similar tridiagonal structure. To solve the eigenvalue problem of Eq. (40) we used exact eigensolvers for dense matrices [21, 22]. Once all the eigenvalues $\{s_\alpha\}$ and eigenvectors $\{r_\alpha\}$ were obtained, we used Eq. (30) to calculate the heat current. We implemented all our programs in a regular desktop computer and were able to solve systems with up to 8000 sites. This amounts to diagonalizing dense matrices of 256×10^6 elements. We did not exploit the sparsity nor the slab structure of the model to simplify the numerical calculation. Therefore, our method can be used also for systems with arbitrarily complex interactions where transfer-matrix methods like the one used in [12] are not viable. Certainly, a more elaborate implementation of our algorithms would enable the study of larger systems.

Figure 1 shows how the heat flux scales with system size for 3D crystals of N^3 sites with $N = 3, 4, 6, 8, 12, 16, 20$. The results are obtained for $k_0 = 10$ and $\Delta = 0.2$, which are the ones used in [12]. The points and error bars correspond to the mean value and the dispersion of the heat current obtained for several disorder realizations. We observe that for strong coupling ($\gamma_0 = .5$, which is consistent with the value used in [12]) the heat flux decrease with the size of the system. The functional form of this dependence is well described by a power law with exponent close to $\mu = -0.86$. However, as shown in Fig. 1 this value is very sensitive to the coupling strength. Thus, for weak coupling ($\gamma_0 = 10^{-3}$) the heat flux does not seem to depend on the system size

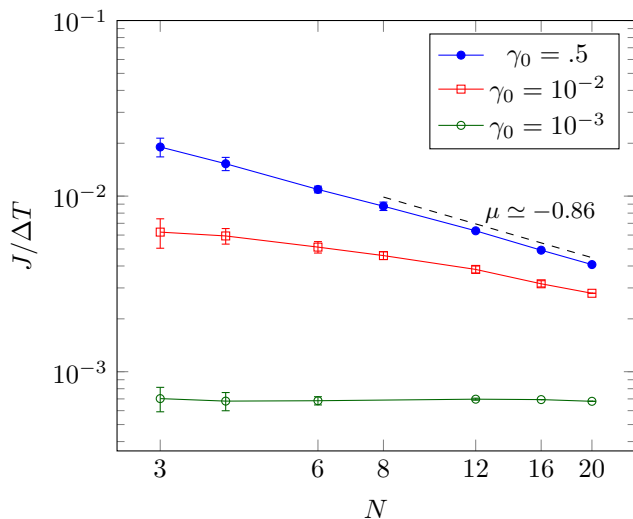


FIG. 1: (Color online) Heat flux vs N in 3D disordered crystals for different values of the coupling constant γ_0 . The parameters are $k_0 = 10$ and $\Delta = 0.2$.

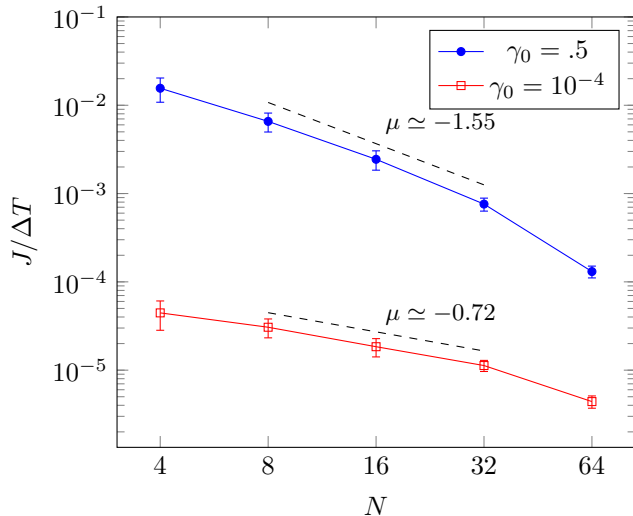


FIG. 2: (Color online) Heat flux vs N in 2D disordered crystals for different values of the coupling constant γ_0 . The parameters are $k_0 = 10$ and $\Delta = 0.2$.

(i.e., in this case we find $\mu = 0$). Therefore, we conclude that the effect of disorder in the mass matrix is qualitatively different in the weak coupling limit (where the normal modes are similar to those of the closed system) in comparison to the strong coupling regime (where the normal modes come from a genuine quadratic eigenvalue problem). The results reported in [12] correspond to the strong coupling regime, and the authors report a power law behavior with an exponent close to $\mu = -1$ (i.e., consistent with Fourier's law) for the same system we analyzed here. Figure 2 shows the scaling of the heat current for 2D square crystals. We see that the exponent μ also depends on the coupling strength, although

the difference between strong and weak coupling is not as dramatic as in the 3D case.

It is important to remark that the results presented here are not conclusive regarding the scaling of the heat current in the thermodynamic limit ($N \rightarrow \infty$). In that limit the exponent μ may turn out to be independent of γ_0 , at least for a reasonable range of values of this coupling constants. However, our results show that for moderately small systems such as the ones analyzed here and in [12], this is not the case. Results for larger systems are needed to clarify this point and to validate a power-law behavior.

As a final comment, we think that the weak coupling limit is more appropriate than the strong coupling regime to discuss the validity or the emergence of the Fourier's law, since in the strong coupling regime the distinction between system and reservoirs is not well defined.

VI. DISCUSSION

We have developed a new method to obtain the asymptotic state of an arbitrary harmonic network connected to Ohmic reservoirs. The method enables us to express the two-point correlations in the asymptotic state in terms of the eigenvalues and eigenvectors of a generalized cubic eigenvalue problem. As the method is valid for any coupling strength and Ohmic spectral densities of arbitrary cutoff, it can be used to study non equilibrium phenomena beyond the weak coupling and Markovian approximations. We also obtained similar exact formulae to calculate the heat current entering or leaving any of the reservoirs connected to the network. The results presented are also useful from a computational point of view, since we were able to solve analytically some integrals that are often evaluated numerically (which for systems of moderate size is neither efficient nor accurate).

We showed how the complexity of the problem can be reduced by using the high cut-off and weak coupling approximations. In this way we were able to recover known results and to provide a general proof of anomalous heat transport, valid for arbitrary symmetric networks in the weak coupling limit.

Our method can be easily generalized to other situations not treated here. For example, the same techniques can be used to calculate the asymptotic state when the reservoirs have spectral densities with different cutoff or are coupled to the network with different strengths. In addition, it is also possible to generalize our results to the case in which the environmental spectral densities are sub-Ohmic or super-Ohmic. The framework also allows the study of quantum correlations (entanglement or quantum discord) in large networks and non-equilibrium settings. These situations will be treated elsewhere.

As a first application, we applied our method to the already studied problem of heat transport in disordered harmonic crystals. We complemented previous results showing that the scaling of the heat current with the sys-

tem size greatly depends on the strength of the coupling between system and reservoirs.

We gratefully acknowledge support of grants from CONICET, UBACyT and ANPCyT.

Appendix A: Green's function and the cubic eigenvalue problem

In this appendix we show how to obtain an analytic expression for the Green's function in terms of eigenvalues and eigenvectors of a linear problem. As explained in the main text, the goal is to calculate $g(s)^{-1}$ where:

$$g(s) = s^3 M + s^2 \Lambda M + s(V + \Delta V) + \Lambda(V - \Delta V) \quad (\text{A1})$$

We recall that Λ is a positive constant and V , ΔV and M are positive-definite symmetric matrices. We will relate $g(s)^{-1}$ to the eigenvalues and eigenvectors of the cubic eigenvalue problem defined by $g(s)$, i.e, to the complex numbers $\{s_\alpha\}$ and vectors $\{r_\alpha\}$ that satisfy:

$$\det(g(s_\alpha)) = 0 \quad \text{and} \quad g(s_\alpha)r_\alpha = 0 \quad (\text{A2})$$

The first step in our derivation is to show that the previous cubic eigenvalue problem can be cast as a linear one. For this we generalize the technique used in [18] to linearize the quadratic eigenvalue problem. First, we note that Eq. (A2) can be rewritten as:

$$(s_\alpha B - A) \begin{bmatrix} r_\alpha \\ s_\alpha r_\alpha \\ s_\alpha^2 r_\alpha \end{bmatrix} = 0 \quad (\text{A3})$$

where the $3K \times 3K$ matrices A and B are :

$$A = \begin{bmatrix} 0 & C_1 & 0 \\ 0 & 0 & C_2 \\ -\Lambda V_- & -V_+ & -\Lambda M \end{bmatrix} \quad B = \begin{bmatrix} C_1 & 0 & 0 \\ 0 & C_2 & 0 \\ 0 & 0 & M \end{bmatrix} \quad (\text{A4})$$

Here, $V_\pm = V \pm \Delta V$ while C_1 and C_2 are arbitrary invertible matrices. Below, we will choose $C_1 = C_2 = \mathbb{1}$, a choice that ensures that B is positive definite.

The equivalence between Eq. (A2) and Eq. (A3) can be verified by a direct calculation. Other choices for A and B are possible. In summary, so far we proved that the generalized eigenvalues s_α are simply the eigenvalues of the linear problem defined by A and B while the generalized eigenvectors r_α can be obtained as the first K components of the eigenvectors of the same linear problem.

The relation between the cubic and linear problems becomes more transparent by noticing the following identity:

$$\begin{bmatrix} g(s) & & \\ & \mathbb{1} & \\ & & \mathbb{1} \end{bmatrix} = E(s)(sB - A)F(s) \quad (\text{A5})$$

where $E(s)$ and $F(s)$ are:

$$E(s) = \begin{bmatrix} V_+ + s(\Lambda + s)M & (\Lambda + s)M & \mathbb{1} \\ & -\mathbb{1} & 0 \\ & 0 & -\mathbb{1} & 0 \end{bmatrix} \quad (\text{A6})$$

$$F(s) = \begin{bmatrix} \mathbb{1} & 0 & 0 \\ s\mathbb{1} & \mathbb{1} & 0 \\ s^2\mathbb{1} & s\mathbb{1} & \mathbb{1} \end{bmatrix}$$

Note that $E(s)$ and $F(s)$ are polynomial matrices on s but nevertheless their determinant is constant and equal to 1. Therefore $\det(g(s)) = \det(sB - A)$, i.e, the characteristic polynomials of the cubic and linear problems are the same and consequently their eigenvalues match.

The inversion of Eq. (A5) leads to the following expression for $g(s)^{-1}$:

$$g(s)^{-1} = \begin{bmatrix} \mathbb{1} & 0 & 0 \end{bmatrix} F(s)^{-1} (sB - A)^{-1} E(s)^{-1} \begin{bmatrix} \mathbb{1} \\ 0 \\ 0 \end{bmatrix} \quad (\text{A7})$$

Since $E(s)^{-1}$ and $F(s)^{-1}$ can be readily calculated from Eq. (A6) it is easy to see that Eq. (A7) can be transformed into:

$$g(s)^{-1} = \begin{bmatrix} \mathbb{1} & 0 & 0 \end{bmatrix} (sB - A)^{-1} \begin{bmatrix} 0 \\ 0 \\ \mathbb{1} \end{bmatrix} \quad (\text{A8})$$

We assume that the matrix $M = sB - A$ is indeed invertible and that we can find matrices L and R such that $L^\dagger B R = \mathbb{1}$ and $L^\dagger A R = S$, where $S_{\alpha,\beta} = s_\alpha \delta_{\alpha,\beta}$. As A is not symmetric, this assumption is not trivial (when A is not diagonalizable, S has a Jordan normal form, a case that will not be treated here as all physically relevant situations can be studied under the above assumption). For simplicity, we also assume that all eigenvalues are non-degenerate (this can be easily relaxed). Then, we can write

$$(sB - A)^{-1} = R(s\mathbb{1} - S)L^\dagger \quad (\text{A9})$$

and consequently:

$$g(s)^{-1} = \begin{bmatrix} \mathbb{1} & 0 & 0 \end{bmatrix} R(s\mathbb{1} - S)^{-1} L^\dagger \begin{bmatrix} 0 \\ 0 \\ \mathbb{1} \end{bmatrix} \quad (\text{A10})$$

$$= \sum_{\alpha=1}^{3K} \frac{r_\alpha l_\alpha^\dagger}{s - s_\alpha}$$

The last identity contains the important result. In such equation, the K component vector r_α is obtained by the first K components of the α -th column of R . Similarly, the K component vector l_α is formed with the last K components of the α -th column of L . The columns of R and L are just the right and left eigenvectors of A . In this way we have expressed the Laplace transform of the non-equilibrium Green's function of a system with K degrees of freedom in terms of the eigenvalues and eigenvectors of a linear problem of size $3K \times 3K$.

Appendix B: Covariance matrix and heat currents in the asymptotic state

The result we obtained above is useful to compute the covariance matrix and, in this way, fully determine the stationary state of the network. However, for this purpose we still need to perform the frequency integrals appearing in Eq. 8 of the main text. First, it is useful to notice that for Ohmic environments with the same cutoff Λ , we can write $\hat{G}(i\omega)\hat{v}(w)\hat{G}(-i\omega) = \frac{2}{\pi}\gamma_0\Lambda^2 g(i\omega)^{-1}A(\omega)g(-i\omega)^{-1}$ with $A(\omega) = \omega \sum_l P_l \coth(\frac{\omega}{2T_l})$. Therefore Eq. (8) can be rewritten as :

$$\begin{aligned} \sigma^{(n,m)} &= \\ &= \frac{2}{\pi}\gamma_0\Lambda^2 \int_0^\infty Re [\omega^{n+m} i^{n-m} g(i\omega)^{-1} A(\omega) g(-i\omega)^{-1}] d\omega \end{aligned} \quad (B1)$$

Let us now analyze the properties of the function $f_{n,m}(\omega) = Re [\omega^{n+m} i^{n-m} g(i\omega)^{-1} A(\omega) g(-i\omega)^{-1}]$ (where $m, n = 0, 1$). This function is such that:

- $f_{n,m}(\omega)$ is an even function of ω .
- $\omega f_{n,m}(\omega) \rightarrow 0$ for $|\omega| \rightarrow \infty$
- $f_{n,m}(\omega)$ is analytic in all the complex plane with the exception of the poles of $\hat{g}^{-1}(i\omega)$, $\hat{g}^{-1}(-i\omega)$, and $A(\omega)$.

Since the integrand is an even function of ω we can extend the integral appearing in Eq. (B1) to negative values of ω :

$$\sigma^{(n,m)} = \frac{\gamma_0\Lambda^2}{\pi} \int_{-\infty}^{\infty} f_{n,m}(\omega) d\omega \quad (B2)$$

The integrand has simple poles at the points $\omega_\alpha = -is_\alpha$ and $\omega_\alpha = is_\alpha$ (poles of $g(i\omega)$ and $g(-i\omega)$, respectively). The poles of $g(i\omega)$ are always in the upper half-plane. Also, the integrand has infinite simple poles at the points $\{\pm i\omega_{n,l}, n \in \mathbb{N}\}$, where $\omega_{n,l} = n\pi 2T_l$ are the Matsubara frequencies corresponding to the temperature T_l . As explained in [23], the proper way to deal with the poles at the points $\{i\omega_{n,l}\}$ is to use the following identity:

$$\coth\left(\frac{\omega}{2T}\right) = \frac{2T}{\omega} - \frac{1}{i\pi} \psi\left(1 - \frac{i\omega}{2\pi T}\right) + \frac{1}{i\pi} \psi\left(1 + \frac{i\omega}{2\pi T}\right), \quad (B3)$$

where ψ is the digamma function. Using Eq. B3 the function $A(\omega)$ can be written as:

$$A(\omega) = A_H(\omega) - A_L(\omega) - A_L(-\omega), \quad (B4)$$

where:

$$\begin{aligned} A_H(\omega) &= \sum_l 2T_l P_l \\ A_L(\omega) &= \frac{\omega}{i\pi} \sum_l P_l \psi\left(1 - \frac{i\omega}{2\pi T_l}\right). \end{aligned} \quad (B5)$$

The decomposition of Eq. (B4) is useful because $A_H(\omega)$ (which correspond to the high temperature approximation) is only a constant and $A_L(\omega)$ is analytic in the upper half-plane. Inserting Eq. (B4) into the integral of Eq. (B2) the following expression is obtained:

$$\sigma^{(n,m)} = \sigma_H^{(n,m)} - \left(\sigma_L^{(n,m)} + (-1)^{n+m} [\sigma_L^{(n,m)}]^T \right), \quad (B6)$$

where

$$\begin{aligned} \sigma_{H/L}^{(n,m)} &= \\ &= \frac{\gamma_0\Lambda^2}{\pi} Re \left[\int_{-\infty}^{\infty} (i\omega)^n (-i\omega)^m g^{-1}(i\omega) A_{H/L}(\omega) g^{-1}(-i\omega) \right] \end{aligned} \quad (B7)$$

Now, the integrand of the previous expression is analytic in the complex plane with the only exception of the poles of $g^{-1}(i\omega)$. Since $g^{-1}(\omega) \propto \omega^{-3}$ for $|\omega| \rightarrow \infty$ it is possible to choose a closed integration path in the complex plane such that the contribution at infinity vanishes, and that only encloses the poles of $g(i\omega)$. This is depicted in Fig. 3. It is thus possible to evaluate the integral of Eq. B7 using the residue theorem. The residue of $g(i\omega)$ at the pole $\omega_\alpha = -is_\alpha$ is $-ir_\alpha l_\alpha^\dagger$, therefore:

$$\begin{aligned} \frac{\pi}{\gamma_0\Lambda^2} \sigma_{H/L}^{(n,m)} &= \\ &= Re \left[\sum_{\alpha=1}^{3K} (i\omega_\alpha)^n (-i\omega_\alpha)^m (-ir_\alpha l_\alpha^\dagger) A_{H/L}(\omega_\alpha) g^{-1}(-i\omega_\alpha) \right] \end{aligned} \quad (B8)$$

At this point the spectral decomposition of Eq. A10 can be used to expand $g^{-1}(-i\omega)$. In this way we arrive at Eq. 20 of the main text, which is our final result.

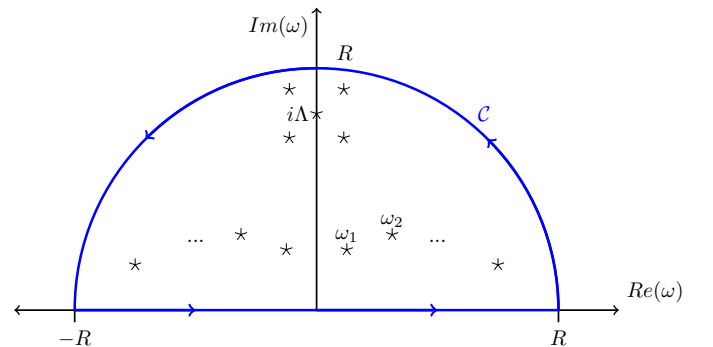


FIG. 3: (Color online) Integration path and poles of $g(i\omega)$.

One possible way to obtain the heat currents is to use the position-momentum covariance matrix $\sigma^{(0,1)}$ and then evaluate the heat current of the l -th reservoir as $\dot{Q}_l = Tr(P_l V_R \sigma^{(0,1)})$. Another possibility is to solve the integral in Eq. (14) of the main text using the same ideas

as before. We find that $\dot{Q}_l = \sum_{l' \neq l} \dot{q}_{l,l'}$, with:

$$\dot{q}_{l,l'} = [2\gamma_0\Lambda^2]^2 \sum_{\substack{\alpha,\beta=1 \\ \omega_\alpha \neq i\Lambda}}^{3K} \frac{\omega_\alpha^3 \Delta_{l,l'}(\omega_\alpha)}{\omega_\alpha^2 + \Lambda^2} \frac{(l_\beta^\dagger P_l r_\alpha)(l_\alpha^\dagger P_{l'} r_\beta)}{\omega_\alpha + \omega_\beta}, \quad (\text{B9})$$

where:

$$\Delta_{l,l'}(\omega) = i \frac{2(T_l - T_{l'})}{\omega} - \frac{2}{\pi} \left[\psi \left(1 - \frac{i\omega}{2\pi T_l} \right) - \psi \left(1 - \frac{i\omega}{2\pi T_{l'}} \right) \right] \quad (\text{B10})$$

Note that in Eq. (B9) the index α does not run over the poles equal to $i\Lambda$. The contribution of these poles vanishes if there are no environments in contact with the same sites of the network, i.e, if $P_l P_{l'} = 0$ for $l \neq l'$. This was assumed in the derivation of Eq. B9. An-

other assumption of the previous results is that there are no poles $\omega_\alpha = -is_\alpha$ with null imaginary part. This is equivalent to assume that all the normal modes of the system suffer dissipation. If some normal models are not in effective contact with the environments and do not suffer dissipation then they can be treated independently as free oscillators. In that case the asymptotic state will be time dependent, and will conserve information about the initial state of the system.

To finish this section we discuss the typical distribution of poles. It is easy to see that if $\text{rank}(\sum_l P_l) < K$ then $i\Lambda$ will be a pole of $g(i\omega)$. This is because $g(-\Lambda) = -2\gamma_0\Lambda^2 \sum_l P_l$ and if $\sum_l P_l$ is not full-rank then $\det(g(-\Lambda)) = 0$. Furthermore, the multiplicity of this root will be $K - \text{rank}(\sum_l P_l)$. For moderate coupling γ_0 there are another $\text{rank}(\sum_l P_l)$ poles close to $i\Lambda$ but with nonzero real part. A typical distribution of poles is depicted in Fig. 3.

-
- [1] Esteban A Martinez and Juan Pablo Paz. Dynamics and thermodynamics of linear quantum open systems. *Physical review letters*, 110(13):130406, 2013.
 - [2] Juan Pablo Paz and Wojciech Hubert Zurek. Environment-induced decoherence and the transition from quantum to classical. In *Fundamentals of Quantum Information*, pages 77–148. Springer, 2002.
 - [3] Amir O Caldeira and Anthony J Leggett. Path integral approach to quantum brownian motion. *Physica A: Statistical mechanics and its Applications*, 121(3):587–616, 1983.
 - [4] Ronnie Kosloff. Quantum thermodynamics: A dynamical viewpoint. *Entropy*, 15(6):2100–2128, 2013.
 - [5] Lorenza Viola, Emanuel Knill, and Seth Lloyd. Dynamical decoupling of open quantum systems. *Phys. Rev. Lett.*, 82:2417–2421, Mar 1999.
 - [6] T. Pellizzari, S. A. Gardiner, J. I. Cirac, and P. Zoller. Decoherence, continuous observation, and quantum computing: A cavity qed model. *Phys. Rev. Lett.*, 75:3788–3791, Nov 1995.
 - [7] M. J. Kastoryano, F. Reiter, and A. S. Sørensen. Dissipative preparation of entanglement in optical cavities. *Phys. Rev. Lett.*, 106:090502, Feb 2011.
 - [8] Hanna Krauter, Christine A. Muschik, Kasper Jensen, Wojciech Wasilewski, Jonas M. Petersen, J. Ignacio Cirac, and Eugene S. Polzik. Entanglement generated by dissipation and steady state entanglement of two macroscopic objects. *Phys. Rev. Lett.*, 107:080503, Aug 2011.
 - [9] Christine A. Muschik, Eugene S. Polzik, and J. Ignacio Cirac. Dissipatively driven entanglement of two macroscopic atomic ensembles. *Phys. Rev. A*, 83:052312, May 2011.
 - [10] Bei Lok Hu, Juan Pablo Paz, and Yuhong Zhang. Quantum brownian motion in a general environment: Exact master equation with nonlocal dissipation and colored noise. *Physical Review D*, 45(8):2843, 1992.
 - [11] Z Rieder, JL Lebowitz, and E Lieb. Properties of a harmonic crystal in a stationary nonequilibrium state. *Journal of Mathematical Physics*, 8(5):1073–1078, 1967.
 - [12] Abhishek Chaudhuri, Anupam Kundu, Dibyendu Roy, Abhishek Dhar, Joel L Lebowitz, and Herbert Spohn. Heat transport and phonon localization in mass-disordered harmonic crystals. *Physical Review B*, 81(6):064301, 2010.
 - [13] Abhishek Dhar and Dibyendu Roy. Heat transport in harmonic lattices. *Journal of Statistical Physics*, 125(4):801–820, 2006.
 - [14] Hirotsugu Matsuda and Kazushige Ishii. Localization of normal modes and energy transport in the disordered harmonic chain. *Progress of Theoretical Physics Supplement*, 45:56–86, 1970.
 - [15] Dibyendu Roy and Abhishek Dhar. Heat transport in ordered harmonic lattices. *Journal of Statistical Physics*, 131(3):535–541, 2008.
 - [16] Abhishek Chaudhuri, Anupam Kundu, Dibyendu Roy, Abhishek Dhar, Joel L Lebowitz, and Herbert Spohn. Heat transport and phonon localization in mass-disordered harmonic crystals. *Physical Review B*, 81(6):064301, 2010.
 - [17] SG Das and A Dhar. Landauer formula for phonon heat conduction: relation between energy transmittance and transmission coefficient. *Eur. Phys. J. B*, 85(11):372, 2012.
 - [18] Françoise Tisseur and Karl Meerbergen. The quadratic eigenvalue problem. *SIAM review*, 43(2):235–286, 2001.
 - [19] A Asadian, D Manzano, M Tiersch, and HJ Briegel. Heat transport through lattices of quantum harmonic oscillators in arbitrary dimensions. *Physical Review E*, 87(1):012109, 2013.
 - [20] Hiroshi Nakazawa. On the lattice thermal conduction. *Progress of Theoretical Physics Supplement*, 45:231–262, 1970.
 - [21] E. Anderson, Z. Bai, C. Bischof, S. Blackford, J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, and D. Sorensen. *LAPACK Users' Guide*. Society for Industrial and Applied Mathematics,

- Philadelphia, PA, third edition, 1999.
- [22] Eric Jones, Travis Oliphant, Pearu Peterson, et al. SciPy: Open source scientific tools for Python, 2001–. [Online; accessed 2014-08-12].
- [23] Peter Riseborough, Peter Hanggi, and Ulrich Weiss. Exact results for a damped quantum-mechanical harmonic oscillator. *Phys. Rev. A*, 31:471–478, Jan 1985.